

A Method to Load Tellurium in Liquid Scintillator to Study Neutrinoless Double Beta Decay

(paper in progress)

The SNO+ Collaboration

A method for loading tellurium into organic liquid scintillator has been developed based on the formation of soluble organic compounds derived from telluric acid ($\text{Te}(\text{OH})_6$, hereafter TeA) and 1,2-butanediol (BD) in conjunction with *N,N*-dimethyldodecylamine (DDA), which acts as a stabilisation/solubilisation agent. The chemicals involved can all be purified to high levels, have high flash points and are relatively safe to work with in underground environments. The loading process results in acceptable optical absorbance and light output in larger detectors for loading levels up to several percent Te by weight. Stability of the loading has been demonstrated to be at least on the timescale of years. Two variants of the loading method are presented below, each resulting in slightly different LAB-soluble mixtures of tellurium compounds with different fluorescence quenching properties.

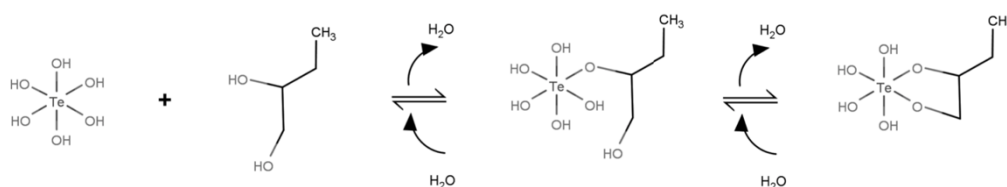


Fig 1: Equilibrium between condensation and hydrolysis reactions in water at room temperature.

When BD is added to dilute aqueous solutions of TeA at room temperature, condensation reactions lead to the attachment of up to two bidentate BD ligands for each tellurium center. This condensation process is in equilibrium with hydrolysis reactions, as indicated in figure 1. At higher concentrations of TeA, the environment is more acidic. This tends to drive the equilibrium in the direction of hydrolysis. The balance can be tipped back towards condensation by adding DDA or heat to the system. Either approach thus leads to the formation of precursor compounds that form the basis for diol-loading of tellurium. Solubilisation in LAB can then be accomplished by removing water after either 1) adding additional heat to form more complex oligomers (TeBD1) through further condensation reactions or 2) using an amine such as DDA for neutralisation in water and to then ionically associate a long carbon chain with the precursor compounds (TeBD2) for solubility in LAB.

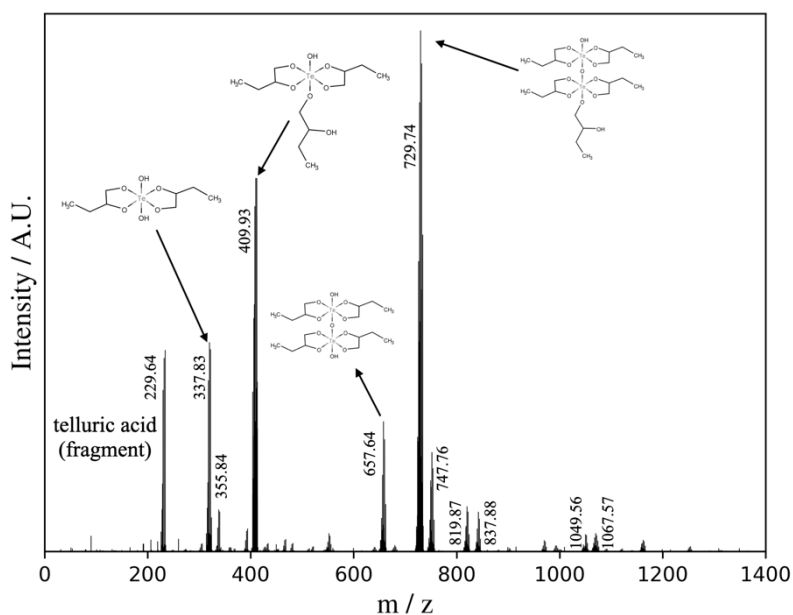


Fig 2: ESI mass spec of TeBD1 compounds in LAB, with possible structures for the main peak identified.

The stability of TeBD1 in scintillator can be dramatically improved by the introduction of DDA. The principle solubilisation mechanism is believed to be the formation of an association between OH groups in the Te compounds and DDA, effectively adding a long carbon tail to the compounds, thereby promoting solubility in LAB and inhibiting further oligomerisation. The de-protonation of the acidic oligomers by the amine has the added benefit of reducing the fluorescence quenching in the scintillator. Based on observations of the light yield, the optimal molar ratio of DDA to Te appears to be very close to 0.5:1.

Neutralisation and solubilisation of the precursor compounds in LAB can be accomplished by first adding DDA to the initial reaction mixture with a molar ratio of 0.5:1:2 for DDA:TeA:BD. In this case, formation of the compounds shown in Fig 3 happen even in the absence of heat and that compound is then directly solubilised into LAB via DDA through the ionic association described above without the need for oligomerisation. This "cold synthesis" approach simply requires the removal of water generated by the condensation reactions that take place during compound formation in order to mix with LAB. This can be accomplished, for example, via nitrogen sparging.

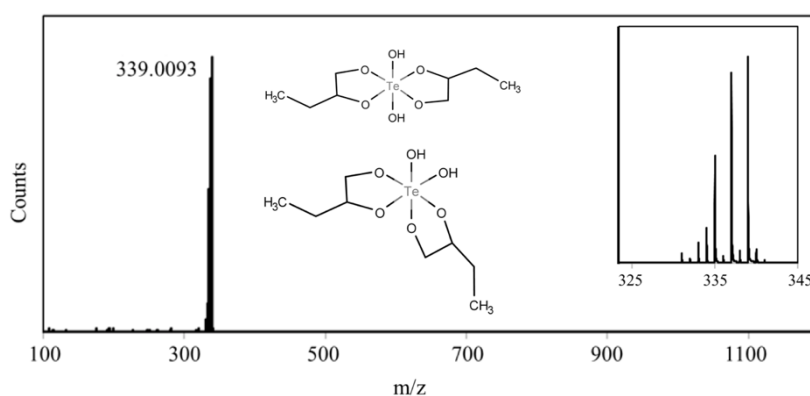


Fig 3: ESI mass spec of TeBD2 compounds in LAB, with corresponding structures identified.

Loading stability of both techniques has been demonstrated on the timescale of at least several years. TeBD2 loading shows reduced fluorescence quenching, permitting practical loading levels of several percent or more of Te by weight in LAB. This is an important advance that opens the door to a highly scalable and economical approach for neutrinoless double beta decay. Further advances in Te loading and associated purification techniques could provide a practical path to realising sensitivity to the non-degenerate normal mass hierarchy.

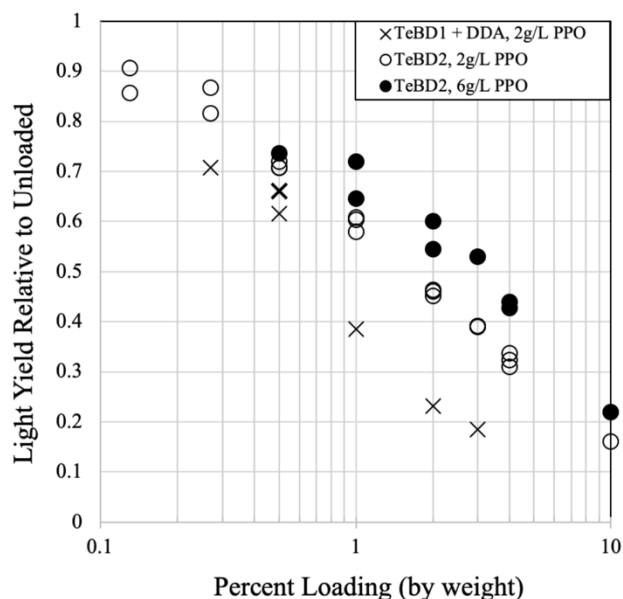


Fig 4: Relative light levels as a function of Te loading for TeBD1 and TeBD2.